MULTISCALE-MULTIPHYSICS MODELLING OF IRRADIATED MATERIALS

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Summary We present a novel multiscale constitutive model to study the mechanical response and internal physical mechanisms of irradiated materials. Radiation defects lead to the performance degradation of the material, irradiation hardening and embrittlement. Understanding the basic mechanisms controlling irradiation effect is crucial for ensuring the safety and reliability of structural components in nuclear reactors and particle accelerator systems. At the atomic scale, Molecular Dynamics simulations are employed to predict the fundamental mechanisms governing the generation, evolution, and interaction of radiation-induced nano-defects under mechanical loads. At the meso- and macroscopic levels, the new, original peridynamic model able to predict the evolution of radiation porosity for ductile material is proposed. The new nonlinear relations of the irradiation hardening based on the atomistic mechanisms are introduced into the constitutive relations. Model is calibrated based on the experimental data obtained during the advanced experimental campaigns dedicated to irradiated materials.

ATOMISITIC STUDY OF PHYSICAL MECHANISMS RESPONSIBLE FOR IRRADIATION-HARDENING

In materials, the displacements of atoms, caused by direct collisions of fast energetic particles with the atoms, are the primary driving force of radiation defects creation. As a result of the collision cascade overlap, the creation of vacancy clusters and/or interstitials clusters occurs. Most of the point defects recombine within the time evolution of the displacement cascade. The remaining defects, voids, cavities, dislocation loops, and stacking-fault tetrahedral (SFTs) form stable defect configurations which are responsible for the radiation-induced microstructural changes, resulting in the evolution of the physical and mechanical properties. Molecular dynamics simulations have proven effective in studying dislocation interactions with inclusions, loops, and voids [1]. An analysis of the sequential interaction of dislocations with individual voids identified a mechanism wherein dislocations cut through voids (Fig. 1: model A), leading to increased void density. Moreover, after the passage of several dislocations, a mechanism of void collapse and dislocation loop formation occurs (Fig. 1: model B), resulting in a coupling effect in the evolution of defects. Model C shown in Fig.1 is based on the process of interaction between a dislocation and a large void, the dislocation on the glide plane absorbs the outermost vacancies from the void, making the void shrink. This model considers the volume change of the void caused by the vacancies absorption and emission during the climb motion of an edge dislocation.

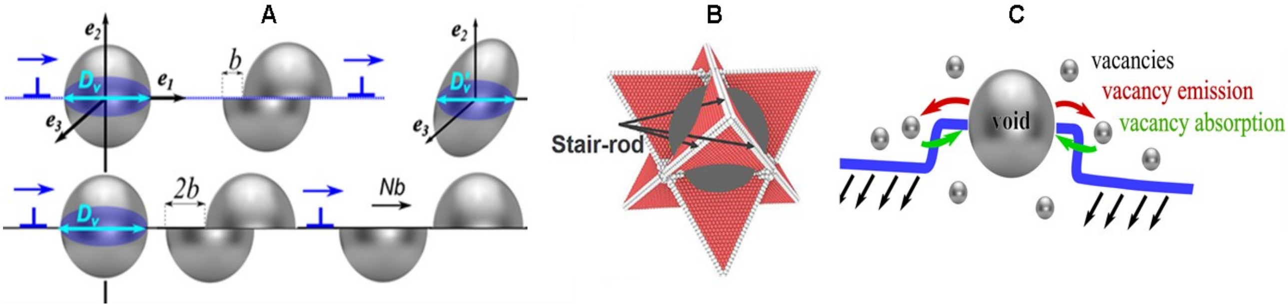

Figure 1. Model A - void cutting; Model B - void collapse; Model C - void shrink

To simulate the evolution of irradiation defects under mechanical loads, irradiated specimens where defects are generated through displacement cascades induced by highly energetic particles were prepared [1]. The shearing tests of irradiated samples compared to the shearing of samples with single defects offer more realistic conditions and a comprehensive understanding of the behaviour of the defective material. During shear deformation, expansion of radiation-induced dislocation loops is observed, and the increase of loop radius, growth, rearrangement and increase in density (Fig. 2). Irradiation-induced loops act as sites for dislocation nucleation during plastic deformation. Moreover, voids can also collapse to form dislocation loops, contributing to plastic flow.

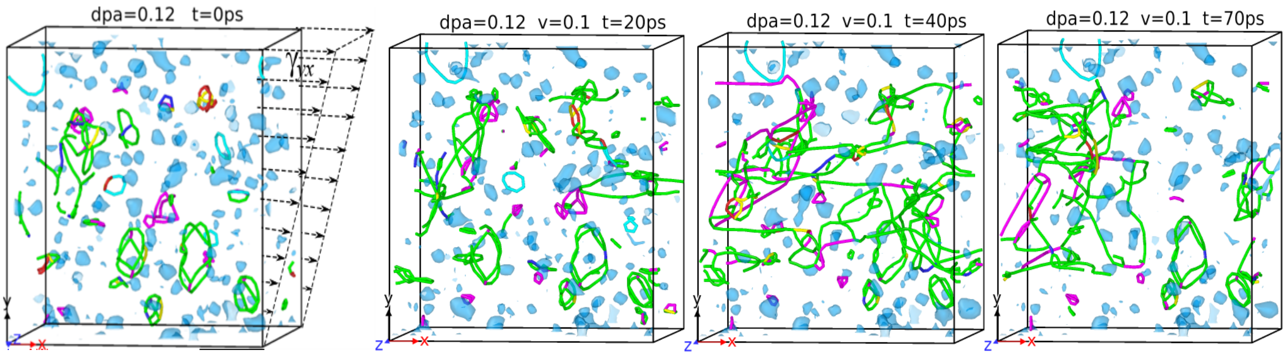

Figure 2. Structural evolution of irradiated samples to 0.12dpa during shear with rate 0.1Å/ps

PERIDYNAMIC ELASTO-PLASTIC DAMAGE MODEL FOR IRRADIATED MATERIALS

At the macroscopic levels, the original peridynamic pressure-dependent constitutive model able to predict the evolution of radiation-induced porosity under mechanical loads is proposed [2]. The definition of radiation porosity is introduced as a volume of discontinuities created in the volume of peridynamic particles (Fig. 3: A). The physical relevance of coupling the porosity with the nonlinear irradiation hardening is discussed. The new physically based constitutive relations for irradiation hardening determined from the dilatational part of elastic strain energy are formulated. The advanced constitutive model considers fully coupled dissipative phenomena in the irradiated material. The peridynamic elasto-plastic model includes coupling the volumetric damage parameter with the yield function. This formulation is kept based on the Gurson model [3]. In addition, peridynamic damage of material is characterized by the reduction of effective force transmission capacity caused by the coupling effect of the damage evolution and the bond elongation increment. Moreover, the hardening and softening rules are introduced to control the evolution of the yield function. The nonlinear irradiation hardening and softening are coupled with the porosity variation (Fig. 3: B, C, D). This coupling effect results in an overall hardening and softening behaviour, owing to the combined effects of both damage and plasticity.

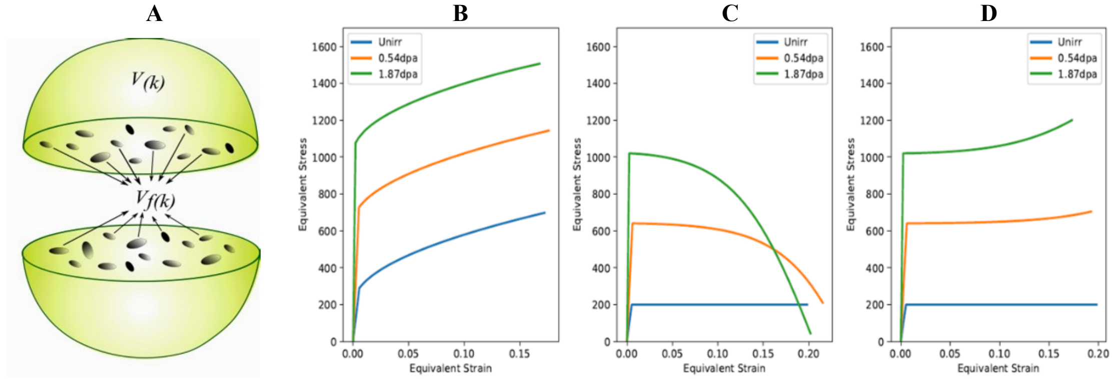

Figure 3. Evolution of the equivalent HMH stress as a function of equivalent plastic strain with selected B) isotropic hardening C) porosity-based softening D) irradiation hardening for different initial level of irradiation

For non-irradiated materials, a strain hardening regime is observed, which is related to the interaction among dislocations (Fig. 3: B). Dislocation motion is impeded by the presence of obstacles in the form of forest dislocations acting as random obstacles. The increase of the initial yield point results directly from the increase of irradiation dose. The dislocations dynamics is controlled by the annihilation process reducing the dislocation density during the plastic deformation (Fig. 3: C). During the interaction of dislocation with voids and loops, voids can divide, loops can collapse, and the dislocations can dissociate into partial dislocations. The third part (Fig. 3: D) describes the mechanisms responsible for softening. The unpinning term is introduced based on the observation that larger radiation obstacles require higher stress to unpin.

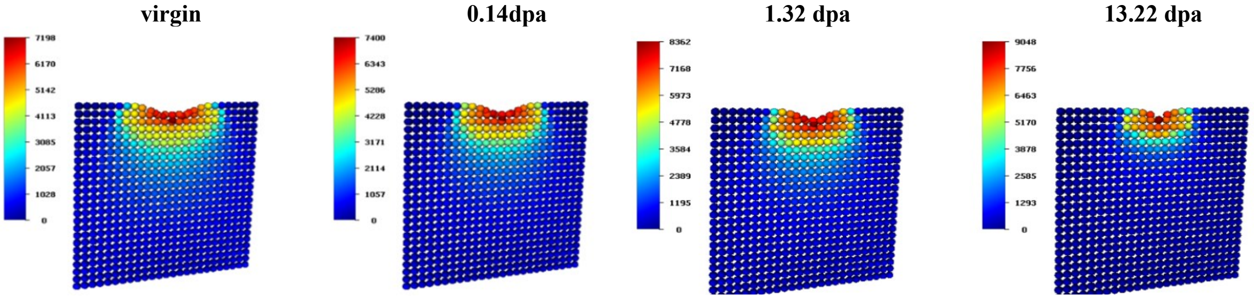
virgin **0.14dpa** **1.32 dpa** **13.22 dpa**

Figure 4. Distribution of equivalent HMH stress at maximum indentation depth for several levels of *dpa*

The distribution of equivalent HMH stress at maximum indentation depth for different values of *dpa* is shown in Fig. 4. With an increasing dose of radiation, the material's initial yield and stiffness increase. Consequently, larger forces have to be applied to achieve the material's plastic behaviour. As expected, the greatest stress values are located in the vicinity of the indenter tip. With increasing *dpa*, the stress level also increases causing the growth of porosity.

EXPERIMENTAL CHARACTERISATION

Ion irradiation campaigns using tandem accelerator were carried out to mimic the effects of neutron irradiation. Validation of the molecular dynamics simulations was performed through transmission electron microscopy (TEM) analyses [1]. A series of indentation experiments were conducted to elucidate the effects of material structure modification and assess the hardening effect originating from radiation defects [2]. The peridynamic predictions are calibrated based on the experimental data to verify the validity of the proposed constitutive model.

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References

[1] Ustrzycka A., Dominguez-Gutierrez J., Chromiński W. Atomisitic study of physical mechanisms responsible for irradiation-hardening in Fe-Ni-Cr alloy. (under review).

[2] Nowak M., Mulewska K., Azarov A., Kurpaska Ł., Ustrzycka A. A peridynamic elasto-plastic damage model for ion-irradiated materials. IJMS. **107806**: 1-46, 2022.

[3] Skoczeń B., Ustrzycka A. Kinetics of evolution of radiation induced micro-damage in ductile materials subjected to time-dependent stresses. *IJP*. **80**: 86-110, 2016.